



chain nodes :

13 14 15 16 17 18 19 20 21 22 23 24 25 27 28

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

6-13 8-16 13-14 14-15 15-21 15-22 16-17 16-23 17-18 18-19 18-20 22-23 23-25 23-24

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

15-21 15-22 16-17 18-19 18-20 22-23

exact bonds :

6-13 8-16 13-14 14-15 16-23 17-18 23-25 23-24

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

G1:MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,PhO,N

G2:C,O

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 27:CLASS 28:CLASS 29:Atom 30:Atom